# Miroslav Medved

## List of Publications by Citations



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|---|---|---|---|
| 77 papers | 1,305 citations | 18 h-index | 32 g-index |
| 78 ext. papers | 1,603 ext. citations | 6.4 avg, IF | 4.59 L-index |

| # | Paper | IF | Citations |
|---|---|---|---|
| 77 | First hyperpolarizability of polymethineimine with long-range corrected functionals. *Journal of Chemical Physics*, **2007**, 126, 191108 | 3.9 | 151 |
| 76 | Mixed-Valence Single-Atom Catalyst Derived from Functionalized Graphene. *Advanced Materials*, **2019**, 31, e1900323 | 24 | 76 |
| 75 | Shedding Light on the Photoisomerization Pathway of Donor-Acceptor Stenhouse Adducts. *Journal of the American Chemical Society*, **2017**, 139, 15596-15599 | 16.4 | 63 |
| 74 | Nonlinear optical properties of ferrocene- and porphyrin-[60]fullerene dyads. *ChemPhysChem*, **2007** , 8, 1056-64 | 3.2 | 62 |
| 73 | A generalized Romberg differentiation procedure for calculation of hyperpolarizabilities. *Computational and Theoretical Chemistry*, **2007**, 847, 39-46 | | 54 |
| 72 | Solvent Effects on the Actinic Step of Donor-Acceptor Stenhouse Adduct Photoswitching. *Angewandte Chemie - International Edition*, **2018**, 57, 8063-8068 | 16.4 | 47 |
| 71 | Reactivity of fluorographene is triggered by point defects: beyond the perfect 2D world. *Nanoscale*, **2018**, 10, 4696-4707 | 7.7 | 45 |
| 70 | Tailoring Photoisomerization Pathways in Donor-Acceptor Stenhouse Adducts: The Role of the Hydroxy Group. *Journal of Physical Chemistry A*, **2018**, 122, 955-964 | 2.8 | 41 |
| 69 | Using Time-Dependent Density Functional Theory to Probe the Nature of Donor-Acceptor Stenhouse Adduct Photochromes. *ChemPhysChem*, **2016**, 17, 1846-51 | 3.2 | 41 |
| 68 | Benchmark calculations of some molecular properties of O2, CN and other selected small radicals using the ROHF-CCSD(T) method. *Molecular Physics*, **2002**, 100, 541-560 | 1.7 | 41 |
| 67 | Iminothioindoxyl as a molecular photoswitch with 100 nm band separation in the visible range. *Nature Communications*, **2019**, 10, 2390 | 17.4 | 34 |
| 66 | 2D Chemistry: Chemical Control of Graphene Derivatization. *Journal of Physical Chemistry Letters*, **2018**, 9, 3580-3585 | 6.4 | 34 |
| 65 | Accuracy assessment of the ROHF□CCSD(T) calculations of static dipole polarizabilities of diatomic radicals: O2, CN, and NO. *Computational and Theoretical Chemistry*, **2001**, 547, 219-232 | | 28 |
| 64 | Dipole moment and polarizability of the low-lying excited states of uracil. *Chemical Physics Letters*, **2012**, 546, 24-29 | 2.5 | 25 |
| 63 | Static NLO responses of fluorinated polyacetylene chains evaluated with long-range corrected density functionals. *Chemical Physics Letters*, **2011**, 515, 78-84 | 2.5 | 23 |
| 62 | Progress and challenges in understanding of photoluminescence properties of carbon dots based on theoretical computations. *Applied Materials Today*, **2021**, 22, 100924 | 6.6 | 23 |
| 61 | First-Principles Simulations of One- and Two-Photon Absorption Band Shapes of the Bis(BF2) Core Complex. *Journal of Physical Chemistry B*, **2016**, 120, 2323-32 | 3.4 | 21 |

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| 60 | CCSD(T) expectation value calculations of first-order properties. *Theoretical Chemistry Accounts*, **1997**, 98, 75-84 | 1.9 | 20 |
| 59 | Solvatochromic Shifts in UV-Vis Absorption Spectra: The Challenging Case of 4-Nitropyridine N-Oxide. *Journal of Chemical Theory and Computation*, **2016**, 12, 1919-29 | 6.4 | 18 |
| 58 | Tunable Synthesis of Nitrogen Doped Graphene from Fluorographene under Mild Conditions. *ACS Sustainable Chemistry and Engineering*, **2020**, 8, 4764-4772 | 8.3 | 17 |
| 57 | Intrinsic photoluminescence of amine-functionalized graphene derivatives for bioimaging applications. *Applied Materials Today*, **2019**, 17, 112-122 | 6.6 | 17 |
| 56 | Alkynylation of graphene via the Sonogashira C-C cross-coupling reaction on fluorographene. *Chemical Communications*, **2019**, 55, 1088-1091 | 5.8 | 15 |
| 55 | Quantifying the Performances of DFT for Predicting Vibrationally Resolved Optical Spectra: Asymmetric Fluoroborate Dyes as Working Examples. *Journal of Chemical Theory and Computation*, **2017**, 13, 4347-4356 | 6.4 | 14 |
| 54 | Linear phosphorus–boron chains: model system with huge electronic first hyperpolarizability. *International Journal of Quantum Chemistry*, **2005**, 103, 226-234 | 2.1 | 14 |
| 53 | Carbon Dots Detect Water-to-Ice Phase Transition and Act as Alcohol Sensors Fluorescence Turn-Off/On Mechanism. *ACS Nano*, **2021**, 15, 6582-6593 | 16.7 | 14 |
| 52 | Solvent Effects on the Actinic Step of Donor–Acceptor Stenhouse Adduct Photoswitching. *Angewandte Chemie*, **2018**, 130, 8195-8200 | 3.6 | 14 |
| 51 | Variability of C–F Bonds Governs the Formation of Specific Structural Motifs in Fluorinated Graphenes. *Journal of Physical Chemistry C*, **2019**, 123, 27896-27903 | 3.8 | 13 |
| 50 | Combined high degree of carboxylation and electronic conduction in graphene acid sets new limits for metal free catalysis in alcohol oxidation. *Chemical Science*, **2019**, 10, 9438-9445 | 9.4 | 13 |
| 49 | Comparison of Property-Oriented Basis Sets for the Computation of Electronic and Nuclear Relaxation Hyperpolarizabilities. *Journal of Chemical Theory and Computation*, **2015**, 11, 4119-28 | 6.4 | 13 |
| 48 | Conformational Behavior and Optical Properties of a Fluorophore Dimer as a Model of Luminescent Centers in Carbon Dots. *Journal of Physical Chemistry C*, **2020**, 124, 14327-14337 | 3.8 | 13 |
| 47 | Exploring the Solvatochromism of Betaine 30 with Ab Initio Tools: From Accurate Gas-Phase Calculations to Implicit and Explicit Solvation Models. *Chemistry - A European Journal*, **2017**, 23, 4108-4119 | 4.8 | 12 |
| 46 | Effect of the leaving group on the reaction of 2-aminopyrroles with electron deficient heteroaromatic azadienes: substitution by addition–elimination versus cycloaddition. *Tetrahedron Letters*, **2007**, 48, 3991-3994 | 2 | 12 |
| 45 | Tailoring π-conjugation and vibrational modes to steer on-surface synthesis of pentalene-bridged ladder polymers. *Nature Communications*, **2020**, 11, 4567 | 17.4 | 12 |
| 44 | Can Density Functional Theory Be Trusted for High-Order Electric Properties? The Case of Hydrogen-Bonded Complexes. *Journal of Chemical Theory and Computation*, **2019**, 15, 3570-3579 | 6.4 | 11 |
| 43 | Direct and indirect effects of dispersion interactions on the electric properties of weakly bound complexes. *Journal of Physical Chemistry A*, **2015**, 119, 3112-24 | 2.8 | 11 |

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| 42 | Full cLR-PCM calculations of the solvatochromic effects on emission energies. *Physical Chemistry Chemical Physics*, **2014**, 16, 26024-9 | 3.6 | 11 |
| 41 | Unveiling solvents effect on excited-state polarizabilities with the corrected linear-response model. *Journal of Physical Chemistry A*, **2014**, 118, 5652-6 | 2.8 | 11 |
| 40 | Electric properties of the low-lying excited states of benzonitrile: geometry relaxation and solvent effects. *Theoretical Chemistry Accounts*, **2015**, 134, 1 | 1.9 | 11 |
| 39 | Theoretical analysis of charge-transfer electronic spectra of methylated benzenes⋯TCNE complexes including solvent effects: approaching experiment. *Theoretical Chemistry Accounts*, **2012**, 131, 1 | 1.9 | 11 |
| 38 | On the physical origins of interaction-induced vibrational (hyper)polarizabilities. *Physical Chemistry Chemical Physics*, **2016**, 18, 22467-77 | 3.6 | 10 |
| 37 | MP2, DFT-D, and PCM study of the HMB⋯TCNE complex: Thermodynamics, electric properties, and solvent effects. *International Journal of Quantum Chemistry*, **2008**, 108, 1533-1545 | 2.1 | 10 |
| 36 | Thermally reduced fluorographenes as efficient electrode materials for supercapacitors. *Nanoscale*, **2019**, 11, 21364-21375 | 7.7 | 10 |
| 35 | Zigzag sp Carbon Chains Passing through an sp Framework: A Driving Force toward Room-Temperature Ferromagnetic Graphene. *ACS Nano*, **2018**, 12, 12847-12859 | 16.7 | 10 |
| 34 | Partitioning of interaction-induced nonlinear optical properties of molecular complexes. I. Hydrogen-bonded systems. *Physical Chemistry Chemical Physics*, **2018**, 20, 19841-19849 | 3.6 | 9 |
| 33 | High second-order NLO responses of dehydrogenated hydrogen cyanide borane(1) oligomers. *Computational and Theoretical Chemistry*, **2010**, 961, 66-72 | | 9 |
| 32 | Molecular Fluorophores Self-Organize into C-Dot Seeds and Incorporate into C-Dot Structures. *Journal of Physical Chemistry Letters*, **2020**, 11, 8252-8258 | 6.4 | 9 |
| 31 | Tunable one-step double functionalization of graphene based on fluorographene chemistry. *Chemical Communications*, **2020**, 56, 1936-1939 | 5.8 | 8 |
| 30 | Tuning the NLO properties of polymethineimine chains by chemical substitution. *Chemical Physics*, **2013**, 415, 196-206 | 2.3 | 8 |
| 29 | Critical analysis of spectral solvent shifts calculated by the contemporary PCM approaches of a representative series of charge-transfer complexes between tetracyanoethylene and methylated benzenes. *Physical Chemistry Chemical Physics*, **2015**, 17, 17618-27 | 3.6 | 8 |
| 28 | EFFECT OF ELECTRON-WITHDRAWING SUBSTITUENTS ON THE INVERSE-ELECTRON DEMAND DIELS-ALDER REACTION OF 2-AMINOPYRROLES AND 1,3,5-TRIAZINES. *Heterocyclic Communications*, **2007**, 13, | 1.7 | 8 |
| 27 | Weakly interacting molecular clusters of CO with H2O, SO2, and NO+. *Molecular Physics*, **2014**, 112, 3225-3236 | 1.7 | 7 |
| 26 | A DFT study of H-isomerisation in alkoxy-, alkylperoxy- and alkyl radicals: Some implications for radical chain reactions in polymer systems. *Polymer Degradation and Stability*, **2011**, 96, 660-669 | 4.7 | 7 |
| 25 | Longitudinal NLO properties of C2H2, HCCF, and C2F2: Electron correlation and vibration effects. *International Journal of Quantum Chemistry*, **2005**, 102, 209-223 | 2.1 | 7 |

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| 24 | Bimodal role of fluorine atoms in fluorographene chemistry opens a simple way toward double functionalization of graphene. *Carbon*, **2019**, 145, 251-258 | 10.4 | 6 |
| 23 | NLO responses of small polymethineimine oligomers: A CCSD(T) study. *Computational and Theoretical Chemistry*, **2007**, 821, 160-165 | | 6 |
| 22 | Covalently Interlinked Graphene Sheets with Sulfur-Chains Enable Superior Lithium–Sulfur Battery Cathodes at Full-Mass Level. *Advanced Functional Materials*, **2021**, 31, 2101326 | 15.6 | 6 |
| 21 | Contribution of the Molecular Fluorophore IPCA to Excitation-Independent Photoluminescence of Carbon Dots. *Journal of Physical Chemistry C*, **2021**, 125, 12140-12148 | 3.8 | 6 |
| 20 | Single-Atom Catalysis: Mixed-Valence Single-Atom Catalyst Derived from Functionalized Graphene (Adv. Mater. 17/2019). *Advanced Materials*, **2019**, 31, 1970125 | 24 | 5 |
| 19 | Optical properties of V-shaped bis-coumarins: Ab initio insights. *Computational and Theoretical Chemistry*, **2016**, 1076, 57-64 | 2 | 5 |
| 18 | Anchoring of Transition Metals to Graphene Derivatives as an Efficient Approach for Designing Single-Atom Catalysts. *Advanced Materials Interfaces*, **2021**, 8, 2001392 | 4.6 | 5 |
| 17 | Solvent Effects on Molecular Electric Properties **2017**, 741-794 | | 4 |
| 16 | Theoretical study (CC2, DFT and PCM) of charge transfer complexes between antithyroid thioamides and TCNE: electronic CT transitions. *Journal of Molecular Modeling*, **2014**, 20, 2312 | 2 | 4 |
| 15 | Enhancement of the second-order NLO responses of boron–nitrogen oligomers by copolymerization with polyyne. *Computational and Theoretical Chemistry*, **2009**, 901, 194-201 | | 4 |
| 14 | Nitrogen doped graphene with diamond-like bonds achieves unprecedented energy density at high power in a symmetric sustainable supercapacitor.. *Energy and Environmental Science*, **2022**, 15, 740-748 | 35.4 | 4 |
| 13 | Tailoring the optical and dynamic properties of iminothioindoxyl photoswitches through acidochromism. *Chemical Science*, **2021**, 12, 4588-4598 | 9.4 | 4 |
| 12 | Theoretical study of charge transfer complexes between antithyroid thioamides and TCNE: Thermodynamics of the complex formation. *Computational and Theoretical Chemistry*, **2015**, 1051, 129-136 | 2 | 3 |
| 11 | Accurate Nonlinear Optical Properties of Solvated -Nitroaniline Predicted by an Electrostatic Discrete Local Field Approach. *Journal of Physical Chemistry B*, **2020**, 124, 10195-10209 | 3.4 | 3 |
| 10 | The behavior of a paramagnetic system in electric and magnetic fields as exemplified by revisiting Li@BH. *Physical Chemistry Chemical Physics*, **2017**, 19, 12229-12236 | 3.6 | 2 |
| 9 | Partitioning of interaction-induced nonlinear optical properties of molecular complexes. II. Halogen-bonded systems. *Physical Chemistry Chemical Physics*, **2020**, 22, 4225-4234 | 3.6 | 2 |
| 8 | MP2 and DFT study of IR spectra of TCNE-methylsubstituted benzene complexes: Is charge transfer important?. *International Journal of Quantum Chemistry*, **2009**, 110, NA-NA | 2.1 | 2 |
| 7 | Electric Properties of Cyanoborane Isomers. *Collection of Czechoslovak Chemical Communications*, **2005**, 70, 1055-1081 | | 2 |

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| 6 | Electric properties of hydrated uracil: From micro- to macrohydration. *Journal of Molecular Liquids*, **2019**, 275, 338-346 | 6 | 2 |
| 5 | Stretch-Healable Molecular Nanofibers. *Advanced Theory and Simulations*, **2020**, 3, 2000094 | 3.5 | 1 |
| 4 | Design of High-Performance Pyridine/Quinoline Hydrazone Photoswitches. *Journal of Organic Chemistry*, **2021**, 86, 11633-11646 | 4.2 | 1 |
| 3 | Accessibility of Grafted Functional Groups Limits Reactivity of Covalent Graphene Derivatives. *Applied Surface Science*, **2022**, 153792 | 6.7 | 1 |
| 2 | Solvent Effects on Molecular Electric Properties **2015**, 1-54 | | 0 |
| 1 | Using Time-Dependent Density Functional Theory to Probe the Nature of Donor-Acceptor Stenhouse Adduct Photochromes. *ChemPhysChem*, **2016**, 17, 1712-1712 | 3.2 | |